

# Theoretical study of X-ray absorption of three-dimensional topological insulator $\text{Bi}_2\text{Se}_3$

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(Dated: January 25, 2013)

X-ray absorption edge singularity which is usually relevant for metals is studied for the prototype topological insulator  $\text{Bi}_2\text{Se}_3$ . The generalized integral equation of Nozières and Dominici type for X-ray edge singularity is derived and solved. The spin texture of surface states causes a component of singularity dependent on the helicity of the spin texture. It also yields another component for which the singularity from excitonic processes is absent.

PACS numbers: 75.70.Tj, 78.20.Bh, 78.67.Wj, 78.70.Dm

**Introduction-** The topological insulators (TI) have been intensively studied recently.<sup>1,2</sup> TI have bulk energy gap but they have conducting (namely gapless) states at *boundary*.<sup>3</sup> Quantum Hall state is an example of 2-dimensional TI with broken time reversal symmetry, and the conducting states at boundary are nothing but the well-known edge states.<sup>3</sup> There exist 3-dimensional TI *with* time reversal invariance, and they have conducting *surface* states (SS) which are protected by  $Z_2$  topological invariants in the bulk.<sup>4-6</sup> The energy band of the SS takes the form of Dirac cone.<sup>1,3</sup> SS have been first observed in  $\text{Bi}_{1-x}\text{Sb}_x$ , but many of their important features were not clearly discerned due to small bulk gap and disorder effect.<sup>7</sup> Stoichiometric TI possessing the simplest SS structure, namely a single Dirac cone, have been proposed for  $\text{Bi}_2\text{Se}_3, \text{Bi}_2\text{Te}_3, \text{Sb}_2\text{Te}_3$ .<sup>8,9</sup> The single Dirac cone SS has been observed in ARPES experiment for  $\text{Bi}_2\text{Se}_3$ .<sup>10</sup> These materials can be realized as TI owing to the band inversion mechanism driven by large spin-orbit coupling.<sup>8</sup> The spin texture which is a distinguished feature of SS has also been observed in the spin-resolved ARPES experiment.<sup>11</sup>

X-ray absorption (and emission) spectroscopy is a very important method in the study of the electronic structure of core electrons. An incident x-ray photon excites a deep core electron to an unoccupied state with higher energy, leaving behind a positively charged core hole which can be treated to be immobile in many cases.<sup>12,13</sup> If there exist conduction electrons (of metals), they react to this *suddenly* created potential by deep core hole. The conduction electrons interact with deep core hole in two distinctive ways: the excitonic process<sup>14</sup> which is essentially attraction between hole and conduction electrons and the orthogonality catastrophe<sup>15</sup> which means a vanishing overlap between the ground-state wavefunctions before and after the creation of the deep core hole. Both excitonic process and orthogonality catastrophe are singular near x-ray absorption edge for fermi liquids, and they require nonperturbative treatments.<sup>16-19</sup> For TI, partially filled SS comprise the conduction electrons in spite of energy gap in the bulk. Evidently, it is of interest to investigate how the above singular behaviors for the conventional fermi liquids are modified for the conducting states realized by SS of TI.

However, there is a caveat. In the X-ray absorption

experiment with photon incident perpendicular to surface, X-rays penetrate deep into the bulk of a sample, hence providing its bulk properties.<sup>20</sup> The SS of TI reside near surface, so that in this experimental setup the contribution to the absorption from SS is expected to be rather small. The decay length (along surface normal) of SS of  $\text{Bi}_2\text{Se}_3$  can be estimated to be in the range of  $4 \sim 10 \text{ \AA}$  using Eq.(32) and Table IV of Ref.[9]. For the substantial amount of X-ray absorption to take place in conjunction with SS the attenuation length of X-ray should be comparable to the decay length of SS. The attenuation length of X-ray can be controlled by its energy and the incident angle (measured from surface). Taking various factors mentioned above into account, we choose to focus on a core level  $\text{N}_{34}\text{p}_{3/2}$  of Bi whose binding energy is 678.8 eV. At this energy the critical angle is 3.26 degrees and the attenuation length at 3.4 degrees is  $40 \text{ \AA}$  which is indeed comparable to the decay length of SS. We note that the attenuation length for the normal incidence is about  $1,000 \text{ \AA}$ .<sup>20</sup> Presently there seems to be no experimental report on the X-ray absorption in  $\text{Bi}_2\text{Se}_3$ .

In this Brief Report we report the results on the X-ray edge problem of  $\text{Bi}_2\text{Se}_3$ . The spin texture structure of SS modifies the singular edge behavior compared to that of conventional Fermi liquids. The most salient differences are the appearance of a contribution depending on the helicity of spin texture and the other which is free of the singularity from excitonic process. The main result of this Brief Report is Eq.(34).

**Setup-** The Hamiltonian for the SS is given by (see Eq.(34) of Ref.[9], and  $\alpha, \beta = \uparrow, \downarrow$  denote spin )

$$H_{\text{SS}} = \sum_{\alpha, \beta = \uparrow, \downarrow} c_{\mathbf{k}\alpha}^\dagger h_{\alpha\beta} c_{\mathbf{k}\beta}, \quad \hat{h} = (h_{\alpha\beta})$$

$$\hat{h} = (\tilde{C}_0 + \tilde{C}_2(k_x^2 + k_y^2))I_2 + \tilde{A}(\sigma_x k_y - \sigma_y k_x), \quad (1)$$

where  $\sigma_{x,y}$  are Pauli matrices acting on spin space ( $I_2$  is a unit matrix) and  $c_{\mathbf{k}\alpha}$  is the destruction operator for SS with wavenumber  $\mathbf{k}$  and spin  $\alpha$ . In Eq.(1) we have ignored the trigonal distortion terms proportional to  $(k_x \pm ik_y)^3$ . The numerical values of the parameters of Eq.(1) which are appropriate for  $\text{Bi}_2\text{Se}_3$  are given by  $\tilde{C}_0 = 3.37 \times 10^{-2} \text{ eV}$ ,  $\tilde{C}_2 = 23.7 \text{ eV} \cdot \text{\AA}^2$ ,  $|\tilde{A}| = 3.30 \text{ eV} \cdot \text{\AA}$ . The Fig.4 of Ref.[9] suggests the wavenumber cutoff be

$k_c \approx 0.1 \text{\AA}^{-1}$ . The energy eigenvalue is given by

$$E_{\pm}(\mathbf{k}) = \tilde{C}_0 + \tilde{C}_2 k_{\parallel}^2 \pm |\tilde{A}| k_{\parallel}, \quad k_{\parallel} = \sqrt{k_x^2 + k_y^2}. \quad (2)$$

When the  $\tilde{C}_2 k_{\parallel}^2$  is much smaller than  $|\tilde{A}| k_{\parallel}$  the Dirac cone structure with apex at  $\mathbf{k} = 0$  is manifest.

The non-interacting Matsubara Green's function of SS can be expressed as (the hat denotes matrix and  $\phi$  is the azimuth angle in x-y plane)

$$\hat{g}(i\epsilon, \mathbf{k}) = I_2 g_d + \left[ (+i)\hat{e}_{12}e^{-i\phi} + (-i)\hat{e}_{21}e^{i\phi} \right] g_o, \quad (3)$$

where  $\hat{e}_{ij}$  is a 2x2 matrix whose only non-vanishing element is 1 at  $(i, j)$  entry, and

$$g_d(i\epsilon, \mathbf{k}) = \frac{i\epsilon + \mu - \tilde{C}_0 - \tilde{C}_2 k_{\parallel}^2}{[i\epsilon + \mu - E_+(\mathbf{k})][i\epsilon + \mu - E_-(\mathbf{k})]},$$

$$g_o(i\epsilon, \mathbf{k}) = \frac{\tilde{A} k_{\parallel}}{[i\epsilon + \mu - E_+(\mathbf{k})][i\epsilon + \mu - E_-(\mathbf{k})]}, \quad (4)$$

where  $\mu$  is the chemical potential, and  $\mu > \tilde{C}_0$  will be assumed (namely, the lower Dirac cone is completely occupied). The interrelation between the spin and the angle in Eq.(3) is nothing but the manifestation of the spin texture of SS.<sup>9</sup> Note that the Green's functions of Eq.(4) are independent of the angle  $\phi$ . The Green's functions summed over wavenumber in the long time limit are given by ( $\tau$  is imaginary time)

$$g_d(\tau) = -\frac{\rho}{\tau}, \quad g_o(\tau) = \text{sgn}(\tilde{A}) g_d(\tau), \quad (5)$$

where  $\rho = Ak_F/4\pi v_F$  is the density of states at Fermi energy ( $A$  is the area of unit cell), and  $v_F$  and  $k_F$  is the Fermi velocity and Fermi momentum, respectively, whose detailed form does not concern us here. Note the sign factor  $\text{sgn}(\tilde{A})$  in Eq.(5), which is the signature of the *helicity* of the spin texture of SS.<sup>9</sup>

The core level  $N_{34p_{3/2}}$  of Bi is labeled by the z-component of the total angular momentum  $J = 3/2$ .

$$H_{\text{hole}} = E_h \sum_{m_J = \pm 3/2, \pm 1/2} b_{m_J}^{\dagger} b_{m_J}, \quad (6)$$

where  $b_{m_J}^{\dagger}$  is the creation operator of the hole.  $E_h$  is the core level energy, and  $\mu + E_h$  is the (unrenormalized) threshold energy for X-ray absorption. The potential created by the deep core hole will be assumed to be spherically symmetric, and for simplicity we will consider the isotropic scattering only, so that the potential scattering matrix element for SS is simplified to<sup>18</sup>

$$V_{\mathbf{k}\mathbf{k}'} = -V_0, \quad V_0 > 0 \text{ is constant.} \quad (7)$$

Then the interaction Hamiltonian between SS and the deep core hole is given by

$$H_{\text{int}} = \sum_{\mathbf{k}, \mathbf{k}'} (-V_0) \left( \sum_{\alpha} c_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}'\alpha} \right) \left( \sum_{m_J} b_{m_J}^{\dagger} b_{m_J} \right), \quad (8)$$

where a suitable cutoff in the wavenumber sum is assumed implicitly. The total Hamiltonian consists of

$$H_{\text{tot}} = H_{\text{SS}} + H_{\text{hole}} + H_{\text{int}}. \quad (9)$$

With the Hamiltonian Eq.(9) the hole quantum number  $m_J$  is conserved, and it implies that the deep core hole Green's function is given by

$$-\langle b_{m_J}(\tau) b_{m_J}^{\dagger}(\tau') \rangle = \delta_{m_J, m_J'} D(\tau - \tau'), \quad (10)$$

where the function  $D(\tau)$  is independent of  $m_J$ . The X-ray absorption intensity  $I(\omega)$  ( $\omega$  is the frequency of the incident X-ray) can be expressed in terms of correlation function [using Eq.(10)] as follows:<sup>21</sup>

$$I(\omega) = \text{Im} \int_0^{\infty} e^{i\omega\tau} F(\tau) \Big|_{i\omega \rightarrow \omega + i\delta},$$

$$F(\tau) = \sum_{\mathbf{k}, \mathbf{k}', \alpha, \beta} \sum_{m_J} M_{\mathbf{q}\lambda}(\mathbf{k}, \alpha | m_J) M_{\mathbf{q}\lambda}^*(\mathbf{k}', \beta | m_J)$$

$$\times F_{\mathbf{k}\mathbf{k}'\alpha\beta | m_J}(\tau),$$

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta | m_J}(\tau) = \langle c_{\mathbf{k}\alpha}(\tau) b_{m_J}(\tau) b_{m_J}^{\dagger}(0) c_{\mathbf{k}'\beta}^{\dagger}(0) \rangle, \quad (11)$$

where  $M_{\mathbf{q}\lambda}(\mathbf{k}, \alpha | m_J)$  is the X-ray transition matrix element from the deep core state  $|m_J\rangle$  to the SS (Bloch state)  $|\mathbf{k}, \alpha\rangle$ , and  $\mathbf{q}$  and  $\lambda$  is the wavenumber and the polarization of the incident X-ray, respectively. In many cases of interest, the wavenumber ( $\mathbf{q}, \mathbf{k}$ ) dependence of the X-ray transition matrix element can be ignored. This is due to the localized nature of the wave function of core electron. In the presence of the strong spin-orbit coupling such as the case of Bi, the electron-photon interaction receives additional contribution from the spin-orbit coupling.<sup>22</sup> The explicit form of the transition matrix element including spin-orbit contribution is

$$M_{\mathbf{q}\lambda}(\mathbf{k}\alpha | m_J) = \int d^3\vec{r} e^{i\mathbf{q}\cdot\vec{r}} \left\{ \frac{(-e)}{m_e} \phi_{\mathbf{k}}^{\dagger} \left[ -i\hbar \vec{e}_{\mathbf{q}\lambda} \cdot \nabla \Psi_{m_J} \right] \right.$$

$$\left. + \frac{\hbar(-e)}{4m_e^2 c^2} \phi_{\mathbf{k}}^{\dagger} \vec{\sigma} \cdot \left[ -\hbar\omega \vec{e}_{\mathbf{q}\lambda} \times \nabla \Psi_{m_J} + \nabla V \times \vec{e}_{\mathbf{q}\lambda} \Psi_{m_J} \right] \right\}, \quad (12)$$

where  $\vec{e}_{\mathbf{q}\lambda}$  is the polarization vector of X-ray and  $V(\vec{r})$  is the periodic crystal potential.  $\phi_{\mathbf{k}}(\vec{r})$  and  $\Psi_{m_J}(\vec{r})$  is the (spinor) Bloch wavefunction of SS and the (spinor) wavefunction of core electron, respectively. The dipole approximation  $e^{i\mathbf{q}\cdot\vec{r}} \approx 1$  will be assumed below.

Correlation functions- The correlation function  $F_{\mathbf{k}\mathbf{k}'\alpha\beta | m_J}(\tau)$  of Eq.(11) can be obtained from

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta | m_J}(\xi, \xi' | \tau_1, \tau_2) = \langle T c_{\mathbf{k}\alpha}(\xi) b_{m_J}(\tau_1) b_{m_J}^{\dagger}(\tau_2) c_{\mathbf{k}'\beta}^{\dagger}(\xi') \rangle \quad (13)$$

by the limiting procedure  $\xi \rightarrow \tau_1 - \tau_c$  and  $\xi' \rightarrow \tau_2 + \tau_c$  ( $\tau_c$  is a short-time cutoff).  $T$  denotes time ordering. For the absorption we have to take  $\tau_1 > \tau_2$ . We employ the equation of motion method of Ref.[19] to derive the integral

equation for  $F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi, \xi'|\tau_1, \tau_2)$ . The conservation of the hole number causes the equation of motion to close on itself,<sup>19</sup> and we find the integral equation

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi, \xi'|\tau_1, \tau_2) = \delta_{\mathbf{k}\mathbf{k}'} g_{\alpha\beta}(\xi - \xi', \mathbf{k}) D(\tau_1 - \tau_2) + \sum_{\mathbf{q}', \gamma} \int_{\tau_2}^{\tau_1} d\tau g_{\alpha\gamma}(\xi - \tau, \mathbf{k}) V_{\mathbf{k}\mathbf{q}'} F_{\mathbf{q}'\mathbf{k}'\gamma\beta|m_J}(\tau, \xi'|\tau_1, \tau_2), \quad (14)$$

where  $g_{\alpha\beta}(\xi, \mathbf{k})$  is the Green's function Eq.(3) in (imaginary) time domain. Decomposing  $F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}$  as follows

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi, \xi'|\tau_1, \tau_2) = G_{\mathbf{k}\mathbf{k}'\alpha\beta}(\xi, \xi'|\tau_1, \tau_2) D(\tau_1 - \tau_2) \quad (15)$$

Eq.(14) becomes the following integral equation:

$$G_{\mathbf{k}\mathbf{k}'\alpha\beta}(\xi, \xi'|\tau_1, \tau_2) = \delta_{\mathbf{k}\mathbf{k}'} g_{\alpha\beta}(\xi - \xi', \mathbf{k}) + \sum_{\mathbf{q}', \gamma} \int_{\tau_2}^{\tau_1} d\tau g_{\alpha\gamma}(\xi - \tau, \mathbf{k}) V_{\mathbf{k}\mathbf{q}'} G_{\mathbf{q}'\mathbf{k}'\gamma\beta}(\tau, \xi'|\tau_1, \tau_2) \quad (16)$$

Eq.(16) is the generalization of Eq.(17a) in Ref.[18] to our case of SS.  $G_{\mathbf{k}\mathbf{k}'\alpha\beta}$  and  $D(\tau_1 - \tau_2)$  of Eq.(15) represents the excitonic processes and the orthogonality catastrophe, respectively.<sup>18</sup> It can be shown that the hole Green's function  $D(\tau_1 - \tau_2)$  can be obtained from the solution of Eq.(16) via parametric integral (see Eq.(21) of Ref.[18] and Eq.(11) of Ref.[19]). Thus once Eq.(16) is solved, we can find X-ray absorption intensity from Eqs.(11,15).

In fact, we need to find the Green's function  $G_{\mathbf{k}\mathbf{k}'\alpha\beta}$  summed over wavenumber weighted by transition matrix element  $M_{\mathbf{q}\lambda}(\mathbf{k}\alpha|m_J)$ . In most cases of simple metals the wavenumber dependence of transition matrix element is ignored. However, in our case such dependence is crucial because, as can be seen in Eq.(3), the spin texture structure is encoded in the angle dependence of Green's function. In view of this we expand the transition matrix element in Fourier series of  $e^{i\phi}$  but we will ignore  $k_{\parallel} = \sqrt{k_x^2 + k_y^2}$  dependence.

$$M_{\mathbf{q}\lambda}(\mathbf{k}\alpha|m_J) \approx \sum_{n=0, \pm 1} e^{in\phi} M_{\mathbf{q}\lambda}^{(n)}(\alpha|m_J), \quad (17)$$

where only  $n = 0, \pm 1$  terms are kept since the higher order contributions will be smaller because they involve higher power of  $k_{\parallel}r$ . Let us define (henceforth time arguments are suppressed for notational clarity)

$$\bar{G}_{\alpha\beta|n,n'} \equiv \sum_{\mathbf{k}, \mathbf{k}'} e^{in\phi} (e^{in\phi'})^* G_{\mathbf{k}\mathbf{k}'\alpha\beta}, \quad (18)$$

where a cutoff in wavenumber sum is implicitly assumed. Applying the definition Eq.(18) to Eq.(3) we find

$$\begin{aligned} \bar{g}_{\alpha\beta|0,0} &= \bar{g}_{\alpha\beta|1,1} = \bar{g}_{\alpha\beta|-1,-1} = \delta_{\alpha\beta} g_d(\tau), \\ \bar{g}_{\alpha\beta|1,0} &= \bar{g}_{\alpha\beta|0,-1} = \delta_{\alpha\uparrow} \delta_{\beta\downarrow} (+i) g_o(\tau), \\ \bar{g}_{\alpha\beta|0,1} &= \bar{g}_{\alpha\beta|-1,0} = \delta_{\alpha\downarrow} \delta_{\beta\uparrow} (-i) g_o(\tau), \\ \bar{g}_{\alpha\beta|1,-1} &= \bar{g}_{\alpha\beta|-1,1} = 0. \end{aligned} \quad (19)$$

Now Eq.(16) can be recast into the following form [ recall Eq.(7) ]

$$\begin{aligned} \bar{G}_{\alpha\beta|n,n'}(\xi, \xi'|\tau_1, \tau_2) &= \bar{g}_{\alpha\beta|n,n'}(\xi - \xi') \\ &+ (-V_0) \int_{\tau_2}^{\tau_1} d\tau \bar{g}_{\alpha\gamma|n,0}(\xi - \tau) \bar{G}_{\gamma\beta|0,n'}(\tau, \xi'|\tau_1, \tau_2) \end{aligned} \quad (20)$$

which are coupled integral equations. Noting the factor  $\bar{g}_{\alpha\gamma|n,0}$  and from Eq.(19), we find the nontrivial solutions (with non-vanishing 2nd term) obtain only for  $n = 0, \pm 1$ .

**Solution of integral equation-** The well-known Nozières and Dominicis (ND) (asymptotic) solution in long time limit is  $[g(\xi) = -\frac{\rho}{\xi} = \text{non-interacting Green's function}]^{18}$

$$G_{\text{ND}}(\xi, \xi'|\tau_1, \tau_2) = \cos^2 \delta g(\xi - \xi') \left[ \frac{(\xi - \tau_2)(\tau_1 - \xi')}{(\tau_1 - \xi)(\xi' - \tau_2)} \right]^{\delta/\pi} \quad (21)$$

which satisfies [ compare with Eq.(20) ]

$$\begin{aligned} G_{\text{ND}}(\xi, \xi'|\tau_1, \tau_2) &= g(\xi - \xi') \\ &+ (-V_0) \int_{\tau_2}^{\tau_1} d\tau g(\xi - \tau) G_{\text{ND}}(\tau, \xi'|\tau_1, \tau_2), \end{aligned} \quad (22)$$

where  $\delta$  is the s-wave scattering phase shift

$$\delta = \tan^{-1}[\pi V_0 \rho]. \quad (23)$$

For  $n = n' = 0$ , using Eq.(19), Eq.(20) is found to reduce to Eq.(22). Hence (time arguments suppressed)

$$\bar{G}_{\alpha\beta|0,0} = \delta_{\alpha\beta} G_{\text{ND}}. \quad (24)$$

Noting Eqs.(5,19) we also find the solutions for  $n' = \pm 1$

$$\begin{aligned} \bar{G}_{\alpha\beta|0,1} &= \delta_{\alpha\downarrow} \delta_{\beta\uparrow} (-i) \text{sgn}(\tilde{A}) G_{\text{ND}}, \\ \bar{G}_{\alpha\beta|0,-1} &= \delta_{\alpha\uparrow} \delta_{\beta\downarrow} (+i) \text{sgn}(\tilde{A}) G_{\text{ND}}. \end{aligned} \quad (25)$$

For other values of  $n'$ ,  $\bar{G}_{\alpha\beta|0n'} = 0$ .

Next consider the case of  $n = 1$ . From the property of  $g_{\alpha\gamma|1,0}$  [see Eq.(19)] the nontrivial solutions obtain only for  $\alpha = \uparrow$ , so that

$$\bar{G}_{\downarrow\beta|1,n'} = \bar{g}_{\downarrow\beta|1,n'}. \quad (26)$$

Now take  $\alpha = \uparrow$ .

$$\begin{aligned} \bar{G}_{\uparrow\beta|1,n'}(\xi, \xi'|\tau_1, \tau_2) &= \bar{g}_{\uparrow\beta|1,n'}(\xi - \xi') \\ &+ (-V_0) \int_{\tau_2}^{\tau_1} d\tau \bar{g}_{\uparrow\downarrow|1,0}(\xi - \tau) \bar{G}_{\downarrow\beta|0,n'}(\tau, \xi'|\tau_1, \tau_2). \end{aligned} \quad (27)$$

If  $n' = -1$ , then from  $\bar{g}_{\uparrow\beta|1,-1} = 0$  and  $\bar{G}_{\downarrow\beta|0,-1} = 0$  [see Eq.(25)], we conclude that

$$\bar{G}_{\uparrow\beta|1,-1} = 0. \quad (28)$$

For the case of  $n' = 0$  of Eq.(27),  $\beta$  should be  $\downarrow$ , otherwise both  $\bar{g}$  and  $\bar{G}$  vanish. Thus

$$\bar{G}_{\uparrow\uparrow|10} = 0 \quad (29)$$

and for  $\beta = \downarrow$ , multiplying both sides of Eq.(27) by  $(-i)\text{sgn}(\tilde{A})$ , we find the equation becomes exactly ND type Eq.(22), so that

$$\bar{G}_{\uparrow\downarrow 10} = (+i)\text{sgn}(\tilde{A})G_{\text{ND}}. \quad (30)$$

Repeating the similar analysis for other cases we obtain

$$\begin{aligned} \bar{G}_{\alpha\beta|0,0} &= \delta_{\alpha\beta}G_{\text{ND}}, \quad \bar{G}_{\alpha\beta|1,-1} = \bar{G}_{\alpha\beta|-1,1} = 0, \\ \bar{G}_{\alpha\beta|11} &= \begin{pmatrix} G_{\text{ND}} & 0 \\ 0 & g_d \end{pmatrix}, \quad \bar{G}_{\alpha\beta|-1-1} = \begin{pmatrix} g_d & 0 \\ 0 & G_{\text{ND}} \end{pmatrix}, \\ \bar{G}_{\alpha\beta|01} &= \bar{G}_{\alpha\beta|-10} = \begin{pmatrix} 0 & 0 \\ -i\text{sgn}(\tilde{A})G_{\text{ND}} & 0 \end{pmatrix}, \\ \bar{G}_{\alpha\beta|10} &= \bar{G}_{\alpha\beta|0-1} = \begin{pmatrix} 0 & i\text{sgn}(\tilde{A})G_{\text{ND}} \\ 0 & 0 \end{pmatrix}. \end{aligned} \quad (31)$$

The leading behavior of the core hole Green's function  $D(\tau)$  can be obtained from the second order linked-cluster expansion.<sup>13</sup> The important contribution turns out to be

$$V_0^2 \int_0^\tau d\xi \int_0^\tau d\xi' \text{Tr} [g^{(0)}(\xi - \xi')g^{(0)}(\xi' - \xi)], \quad (32)$$

where  $g^{(0)}(\xi - \xi') = \sum_{\mathbf{k}} g(\mathbf{k}, \xi - \xi') = g_d(\xi - \xi')\mathbf{I}_2$ . Thus the helicity of the spin texture of SS does not affect the core hole Green's function, so that the situation becomes essentially identical with that of ND solution. The evaluations of the integral of Eq.(32) yields logarithms, which is to be exponentiated in the linked-cluster expansion. Comparing with ND solution we find ( $N_c = 2$ , ( $\uparrow, \downarrow$ ))

$$D(\tau > 0) \sim e^{-\omega_T^* \tau} \frac{1}{(\tau/\tau_c)^{N_c(\delta/\pi)^2}}. \quad (33)$$

$\omega_T^*$  is the renormalized threshold for X-ray absorption.

**Results**—Combining the solutions Eqs.(31,33) with the transition matrix element Eq.(12) we can obtain the result for X-ray absorption intensity. Eq.(12) has two components: one from direct dipole transition and the other from spin-orbit coupling. Dipole transition conserves the spin, so that it is diagonal in spin (namely,  $M_\alpha M_\beta^* \propto \delta_{\alpha\beta}$ . This can be verified explicitly in our case). Then Eq.(31) tells us that only  $\bar{G}_{\alpha\beta|(00),(11),(-1,-1)}$  contribute. Among these,  $G_{\text{ND}}$  includes the singularity from excitonic processes while  $g_d$  does not. The cross term of dipole transition and the spin-orbit contribution allows spin off-diagonal configuration. From Eq.(31) we find that this

contribution is proportional to the helicity  $\text{sgn}(\tilde{A})$ . The above considerations give ( $\Theta(x)$  is step function)

$$I(\omega) \sim \Theta(\omega - \omega_T^*) \left[ c_d'(\omega - \omega_T^*)^{N_c(\delta/\pi)^2} + (c_d + \text{sgn}(\tilde{A})c_o)(\omega - \omega_T^*)^{-2\delta/\pi + N_c(\delta/\pi)^2} \right], \quad (34)$$

where  $c_d', c_d, c_o$  are constants.

**Summary and concluding remarks**—We have studied the X-ray absorption edge singularity of the prototype TI,  $\text{Bi}_2\text{Se}_3$ . For the singularity to exist, gapless conducting states are necessary, and SS provide those. Due to the spin texture of SS, two interesting modifications compared to that of convention metals arise: (1) helicity dependent contribution [ $\text{sgn}(\tilde{A})$  term of Eq.(34)] (2) contribution free of singularity from excitonic process [the first term of Eq.(34)]. These features can be verified experimentally by extracting the surface contributions using the angle and energy dependence of the penetration depth of incident X-ray, and we have also suggested a specific core level appropriate for experiments. The angle and energy dependence of the penetration depth can be also used in distinguishing the helicity effect of TI from that of the conventional Rashba spin-orbit energy bands since the latter reside in the bulk. We mention in comparison that the graphenes have *two* Dirac cones from valley structure, so that its qualitative properties different from those of TI.<sup>23</sup> We also mention that when the Fermi energy crosses the apex of Dirac cone, all of the singularities disappear.<sup>23</sup> However, this situation is not generic for TI and is not elaborated in this Report.

## ACKNOWLEDGMENTS

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(No.2010-0025406) and by Mid-career Researcher Program through NRF grant funded by the Mest (No. 2010-0000179) and by the Special Research Grant of Sogang University. We are grateful to H. Kim for useful comments.

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